



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:58 AM UTC

PDB ID : 1XVD / pdb_00001xvd
Title : Soluble methane monooxygenase hydroxylase: 4-fluorophenol soaked structure
Authors : Sazinsky, M.H.; Lippard, S.J.
Deposited on : 2004-10-27
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

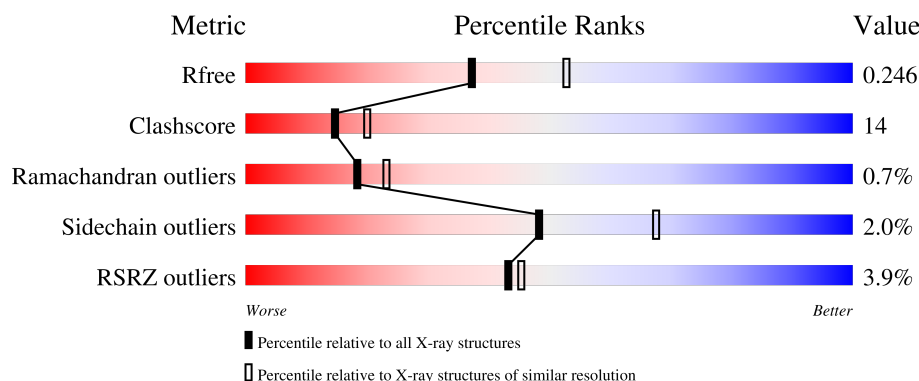
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	527	4% 67% 28% ..
1	B	527	3% 65% 29% ..
2	C	389	78% 19% .
2	D	389	6% 61% 38% .
3	E	170	2% 81% 16% ..

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Mol	Chain	Length	Quality of chain
3	F	170	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	FPN	A	2666	-	X	-	-
5	FPN	B	2667	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18293 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Methane monooxygenase component A alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4148	2655	713	762	18			
1	B	510	Total	C	N	O	S	0	0	0
			4137	2646	711	762	18			

- Molecule 2 is a protein called Methane monooxygenase component A beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	388	Total	C	N	O	S	0	0	0
			3163	2036	545	574	8			
2	D	388	Total	C	N	O	S	0	0	0
			3151	2028	543	572	8			

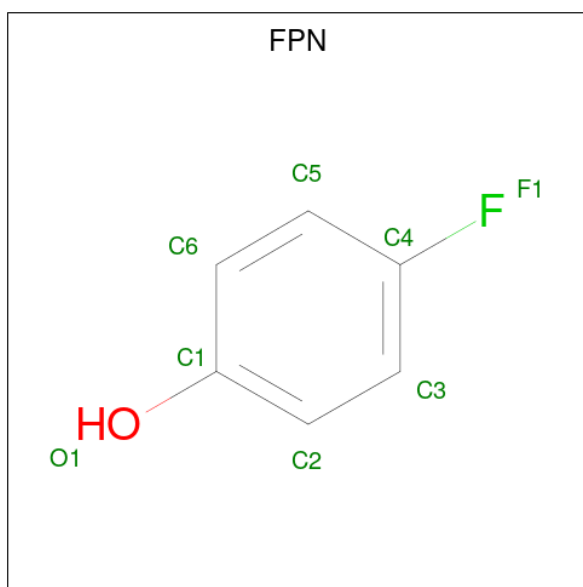
- Molecule 3 is a protein called Methane monooxygenase component A gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	166	Total	C	N	O	S	0	0	0
			1364	864	245	250	5			
3	F	166	Total	C	N	O	S	0	0	0
			1358	860	243	250	5			

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Fe	0	0
			2	2		
4	B	2	Total	Fe	0	0
			2	2		

- Molecule 5 is 4-FLUOROPHENOL (CCD ID: FPN) (formula: C₆H₅FO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	F	O	0	0
			8	6	1	1		
5	B	1	Total	C	F	O	0	0
			8	6	1	1		

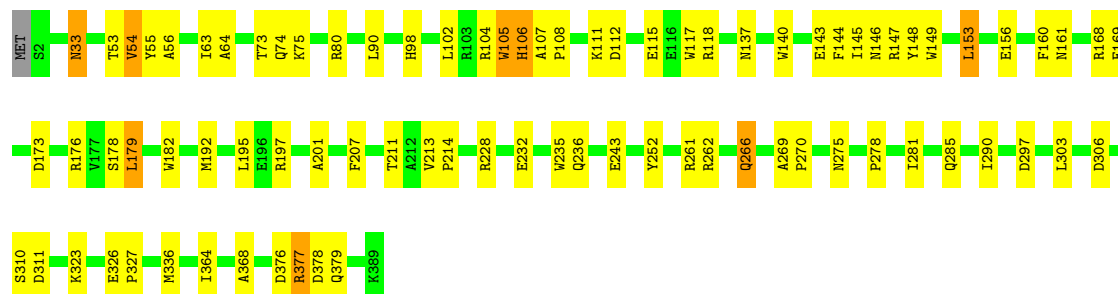
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	200	Total	O	0	0
			200	200		
6	B	198	Total	O	0	0
			198	198		
6	C	277	Total	O	0	0
			277	277		
6	D	105	Total	O	0	0
			105	105		
6	E	124	Total	O	0	0
			124	124		
6	F	48	Total	O	0	0
			48	48		



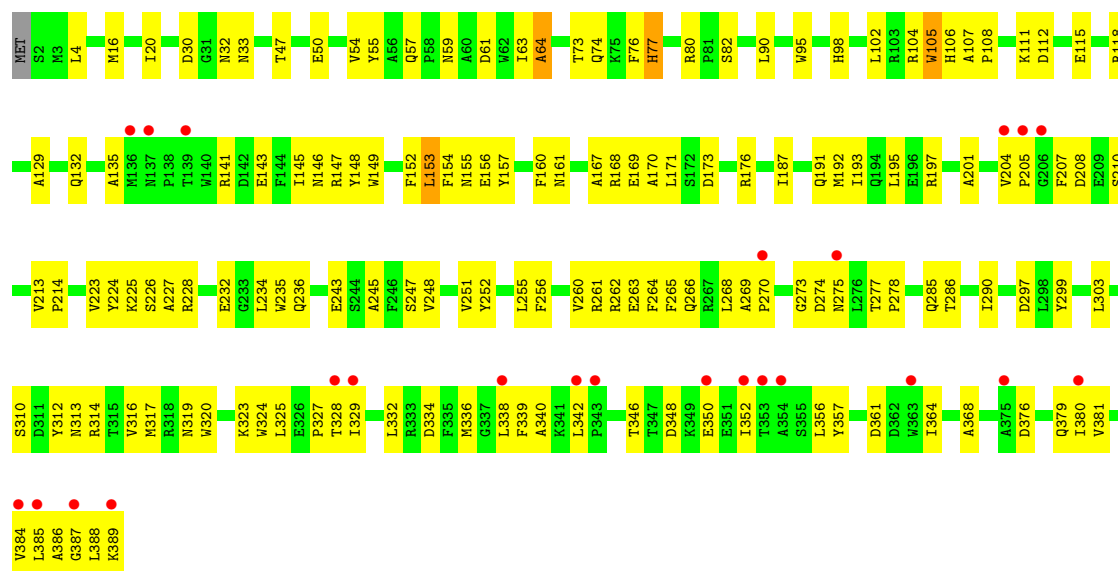
- Molecule 2: Methane monooxygenase component A beta chain

Chain C: 78% 19%



- Molecule 2: Methane monooxygenase component A beta chain

Chain D: 6% 61% 38%



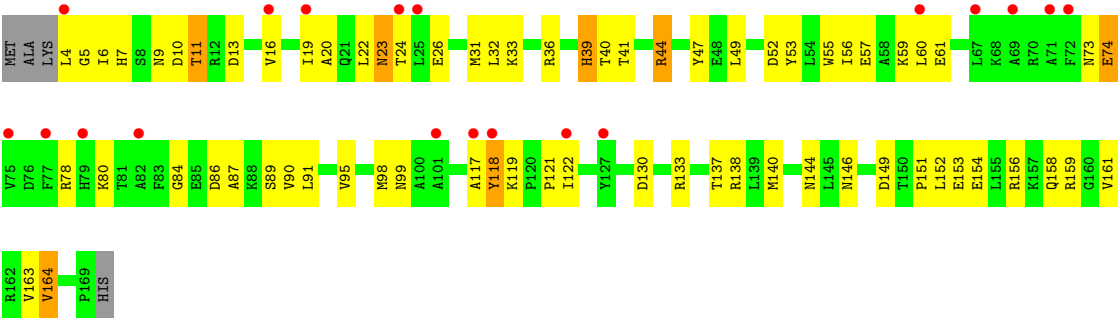
- Molecule 3: Methane monooxygenase component A gamma chain

Chain E: 2% 81% 16%



- Molecule 3: Methane monooxygenase component A gamma chain

Chain F: 11% 57% 36%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.18Å 171.50Å 221.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 2.30 29.94 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.2 (29.94-2.30) 94.3 (29.94-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 2.31Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.194 , 0.229 (Not available) , 0.246	Depositor DCC
R_{free} test set	4028 reflections (3.37%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18293	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FPN, FE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.41	0/4273	0.92	18/5808 (0.3%)
1	B	0.38	0/4262	0.91	16/5796 (0.3%)
2	C	0.44	0/3259	0.90	17/4430 (0.4%)
2	D	0.36	0/3247	0.87	5/4417 (0.1%)
3	E	0.42	0/1392	0.89	7/1876 (0.4%)
3	F	0.34	0/1387	0.86	4/1873 (0.2%)
All	All	0.39	0/17820	0.90	67/24200 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	339	ALA	N-CA-C	9.34	121.22	111.14
3	F	6	ILE	N-CA-C	9.12	119.14	110.30
2	C	106	HIS	N-CA-C	7.71	120.37	111.11
2	C	149	TRP	N-CA-C	-6.77	103.98	111.36
2	C	105	TRP	N-CA-C	-6.56	100.50	110.14
2	D	104	ARG	N-CA-C	6.55	118.95	108.41
2	D	105	TRP	N-CA-C	-6.48	100.39	110.17
1	A	164	ASP	CA-C-N	6.48	126.06	119.19
1	A	164	ASP	C-N-CA	6.48	126.06	119.19
3	E	118	TYR	N-CA-C	6.45	121.94	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	148	TYR	N-CA-C	6.39	118.04	111.14
3	E	39	HIS	N-CA-C	6.31	123.08	113.61
1	B	285	VAL	N-CA-C	6.28	116.43	110.53
1	A	496	ILE	N-CA-C	-6.26	104.64	110.53
1	A	309	VAL	N-CA-C	6.25	116.41	110.53
1	A	213	THR	N-CA-C	6.20	118.55	111.11
1	B	193	ILE	N-CA-C	6.17	119.58	113.53
3	F	118	TYR	N-CA-C	6.12	119.69	112.72
1	A	339	ALA	N-CA-C	6.07	117.59	110.97
1	A	178	GLY	CA-C-N	5.97	125.52	119.19
1	A	178	GLY	C-N-CA	5.97	125.52	119.19
2	C	169	GLU	N-CA-C	5.96	120.71	113.38
3	E	130	ASP	N-CA-C	-5.93	104.89	111.36
1	B	496	ILE	N-CA-C	-5.92	104.96	110.53
1	A	397	ASP	CA-C-N	5.91	125.59	119.56
1	A	397	ASP	C-N-CA	5.91	125.59	119.56
2	D	236	GLN	N-CA-C	5.86	120.43	113.28
1	B	397	ASP	CA-C-N	5.81	125.67	119.28
1	B	397	ASP	C-N-CA	5.81	125.67	119.28
2	C	236	GLN	N-CA-C	5.76	120.47	113.38
2	D	286	THR	N-CA-C	-5.74	105.10	111.36
1	B	164	ASP	CA-C-N	5.72	125.40	119.05
1	B	164	ASP	C-N-CA	5.72	125.40	119.05
3	E	23	ASN	N-CA-C	5.72	120.25	112.88
1	A	426	CYS	CA-C-N	5.69	126.07	119.47
1	A	426	CYS	C-N-CA	5.69	126.07	119.47
1	B	309	VAL	N-CA-C	5.67	115.86	110.42
3	E	73	ASN	N-CA-C	-5.58	102.65	110.35
1	B	243	GLU	N-CA-C	5.58	118.12	111.71
3	E	74	GLU	N-CA-C	5.54	117.31	111.28
1	B	490	SER	N-CA-C	5.53	117.31	111.28
1	A	212	PHE	N-CA-C	5.51	119.68	112.13
2	C	137	ASN	CA-C-N	5.51	125.17	119.05
2	C	137	ASN	C-N-CA	5.51	125.17	119.05
1	A	145	ILE	N-CA-C	-5.49	105.02	111.00
2	C	63	ILE	N-CA-C	-5.49	98.56	107.28
3	E	79	HIS	N-CA-C	5.48	121.74	114.12
2	C	56	ALA	N-CA-C	-5.46	105.49	111.82
1	A	285	VAL	N-CA-C	5.42	116.91	111.00
3	F	53	TYR	N-CA-C	5.40	117.16	111.28
1	B	431	LYS	N-CA-C	-5.39	106.87	113.50
2	C	53	THR	N-CA-C	5.39	120.10	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	LYS	N-CA-C	5.35	117.11	111.28
1	A	205	GLN	N-CA-C	5.33	119.72	111.56
2	C	144	PHE	N-CA-C	5.33	118.94	112.23
1	A	162	GLY	N-CA-C	5.30	120.71	112.60
2	C	104	ARG	N-CA-C	5.29	117.34	109.25
1	B	122	GLY	N-CA-C	-5.27	106.11	112.49
2	D	77	HIS	N-CA-C	-5.18	102.38	110.10
2	C	377	ARG	N-CA-C	5.14	116.88	111.28
2	C	54	VAL	N-CA-C	5.12	116.28	109.37
1	A	291	GLU	N-CA-C	5.09	116.91	111.36
2	C	252	TYR	N-CA-C	5.08	116.51	110.97
1	B	145	ILE	N-CA-C	-5.08	105.59	110.72
2	C	262	ARG	N-CA-C	5.08	119.36	112.04
1	B	162	GLY	N-CA-C	5.07	120.35	112.60
3	F	39	HIS	N-CA-C	5.00	121.80	113.89

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	514	ARG	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4148	0	3919	120	0
1	B	4137	0	3888	147	0
2	C	3163	0	2986	64	0
2	D	3151	0	2960	120	0
3	E	1364	0	1352	18	0
3	F	1358	0	1335	60	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	8	0	5	0	0
5	B	8	0	5	0	0
6	A	200	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	198	0	0	5	0
6	C	277	0	0	1	0
6	D	105	0	0	0	0
6	E	124	0	0	2	0
6	F	48	0	0	0	0
All	All	18293	0	16450	468	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (468) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.31	1.07
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.03	1.01
1:A:184:MET:HE2	1:A:188:PHE:HB2	1.45	0.98
2:D:340:ALA:HA	2:D:389:LYS:HE2	1.47	0.96
1:A:338:ASP:OD2	1:A:433:ALA:HB2	1.70	0.91
3:F:41:THR:O	3:F:44:ARG:HD2	1.71	0.90
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.17	0.89
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.55	0.87
1:A:467:GLN:HG3	6:A:2865:HOH:O	1.76	0.85
1:A:209:GLU:HA	1:A:213:THR:HB	1.58	0.82
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.25	0.82
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.28	0.82
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.77	0.82
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.28	0.82
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.64	0.79
3:F:80:LYS:HE2	3:F:84:GLY:HA2	1.64	0.79
3:F:13:ASP:O	3:F:16:VAL:HG22	1.83	0.77
1:B:209:GLU:HA	1:B:213:THR:OG1	1.85	0.76
1:A:435:THR:CG2	1:A:437:ARG:HE	1.99	0.76
2:C:105:TRP:O	2:C:108:PRO:HD2	1.86	0.76
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.85	0.76
1:B:123:MET:HE3	1:B:197:ALA:HA	1.69	0.75
3:F:4:LEU:HD11	3:F:10:ASP:OD2	1.88	0.73
2:C:146:ASN:ND2	2:C:197:ARG:HH21	1.86	0.73
1:A:227:ASN:HD21	1:A:295:LYS:H	1.36	0.73
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.19	0.72
1:B:406:MET:O	1:B:410:GLU:HG3	1.88	0.72
1:A:513:LYS:O	1:A:514:ARG:C	2.33	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:THR:HG21	1:A:437:ARG:HE	1.55	0.72
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.71	0.71
1:B:477:GLU:OE2	1:B:480:GLU:HG2	1.91	0.70
3:F:80:LYS:CE	3:F:84:GLY:HA2	2.22	0.70
1:B:49:LYS:HD3	3:F:140:MET:HB3	1.74	0.70
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.90	0.70
3:F:153:GLU:H	3:F:153:GLU:CD	1.99	0.69
2:D:153:LEU:C	2:D:153:LEU:HD12	2.18	0.68
3:F:91:LEU:O	3:F:95:VAL:HG23	1.92	0.68
1:A:204:LEU:O	1:A:209:GLU:HG3	1.93	0.68
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.76	0.68
3:E:165:HIS:HE1	3:E:167:GLN:HE21	1.43	0.67
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.76	0.67
1:B:196:ASP:HB2	3:F:140:MET:SD	2.35	0.67
1:B:33:GLN:HA	1:B:131:ALA:HB3	1.77	0.67
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.26	0.66
3:F:52:ASP:O	3:F:56:ILE:HG12	1.96	0.66
1:A:401:GLY:HA2	1:A:515:LEU:HD21	1.78	0.66
2:D:325:LEU:O	2:D:329:ILE:HG12	1.95	0.66
3:F:36:ARG:NH1	3:F:119:LYS:HB3	2.11	0.66
3:E:57:GLU:O	3:E:61:GLU:HG3	1.96	0.66
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.79	0.65
2:C:192:MET:HE2	2:C:192:MET:HA	1.77	0.65
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.79	0.65
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.60	0.65
1:A:349:LEU:HD22	1:A:415:ILE:HD12	1.78	0.65
1:A:109:PHE:O	1:A:112:VAL:HG12	1.97	0.65
1:A:186:ARG:HA	2:C:73:THR:OG1	1.97	0.65
1:A:213:THR:O	1:A:217:ILE:HG12	1.96	0.65
1:B:489:ARG:HD2	1:B:495:LEU:O	1.96	0.65
1:A:175:ARG:HG3	1:A:181:TRP:CD2	2.32	0.64
1:A:227:ASN:ND2	1:A:295:LYS:H	1.95	0.64
3:F:19:ILE:HD12	3:F:20:ALA:N	2.13	0.64
1:A:144:GLU:HA	1:A:144:GLU:OE2	1.98	0.64
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.11	0.64
1:B:38:ASP:O	1:B:39:PHE:HB3	1.97	0.64
2:D:275:ASN:C	2:D:278:PRO:HD2	2.21	0.64
2:D:153:LEU:HD12	2:D:154:PHE:N	2.12	0.64
1:B:23:VAL:HB	2:D:195:LEU:HD11	1.80	0.63
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.46	0.63
1:A:76:GLU:OE1	1:B:76:GLU:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ASN:HD21	1:B:295:LYS:H	1.45	0.63
1:B:402:PHE:C	1:B:403:ILE:HD12	2.23	0.63
1:B:18:ARG:O	2:D:129:ALA:HA	1.98	0.63
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.82	0.62
1:B:193:ILE:HD11	2:D:82:SER:HB3	1.80	0.62
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.83	0.62
1:B:489:ARG:HH11	1:B:496:ILE:HA	1.65	0.62
2:D:348:ASP:OD2	2:D:350:GLU:HB2	2.00	0.62
2:D:245:ALA:HB3	2:D:299:TYR:OH	2.00	0.62
3:F:61:GLU:O	3:F:121:PRO:HG2	2.00	0.61
1:A:160:LYS:HE3	6:A:2857:HOH:O	2.01	0.61
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.96	0.61
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.82	0.61
1:A:108:ASN:HD21	1:A:175:ARG:HE	1.48	0.61
1:B:247:MET:HE2	1:B:247:MET:HA	1.82	0.61
2:D:255:LEU:HD12	2:D:328:THR:HG21	1.83	0.61
2:D:135:ALA:O	2:D:273:GLY:HA3	2.01	0.60
1:A:33:GLN:HA	1:A:131:ALA:HB3	1.83	0.60
1:B:185:LYS:O	1:B:189:SER:HB2	2.02	0.60
1:B:43:ARG:HD2	1:B:43:ARG:C	2.26	0.60
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.83	0.60
2:D:261:ARG:HE	2:D:285:GLN:NE2	2.00	0.60
1:A:116:ASN:CG	1:A:189:SER:HA	2.27	0.60
3:F:90:VAL:HG11	3:F:118:TYR:CE2	2.37	0.60
1:A:401:GLY:HA2	1:A:515:LEU:CD2	2.32	0.59
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.03	0.59
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.85	0.59
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.49	0.59
3:F:57:GLU:O	3:F:61:GLU:HG3	2.02	0.59
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.83	0.59
1:B:49:LYS:HE3	3:F:144:ASN:HD22	1.67	0.59
3:E:41:THR:O	3:E:44:ARG:HD2	2.03	0.58
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.36	0.58
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.69	0.58
2:D:57:GLN:NE2	2:D:59:ASN:HD21	2.02	0.58
2:D:269:ALA:HB1	2:D:274:ASP:OD2	2.04	0.57
3:E:41:THR:O	3:E:44:ARG:CD	2.52	0.57
1:A:108:ASN:ND2	1:A:175:ARG:HH21	2.01	0.57
1:B:188:PHE:HZ	1:B:213:THR:HG22	1.69	0.57
2:D:247:SER:HG	2:D:324:TRP:CD1	2.22	0.57
1:A:108:ASN:HD21	1:A:175:ARG:HH21	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:148:TYR:HE2	2:D:223:VAL:HG21	1.69	0.57
2:D:336:MET:CE	2:D:356:LEU:HD11	2.34	0.57
1:A:406:MET:O	1:A:410:GLU:HG3	2.05	0.57
1:A:185:LYS:O	1:A:189:SER:HB2	2.04	0.57
1:A:140:GLN:O	1:A:144:GLU:HG2	2.05	0.56
1:A:190:ASP:HB3	2:C:74:GLN:O	2.05	0.56
2:C:98:HIS:HE1	2:C:178:SER:OG	1.88	0.56
3:F:9:ASN:OD1	3:F:11:THR:HG23	2.05	0.56
1:B:23:VAL:HB	2:D:195:LEU:CD1	2.35	0.56
1:B:398:PRO:HG3	1:B:507:TRP:CD1	2.40	0.56
1:A:413:HIS:HD2	1:A:428:SER:OG	1.88	0.56
2:D:105:TRP:O	2:D:108:PRO:HD2	2.04	0.56
3:F:130:ASP:OD1	3:F:133:ARG:NH1	2.39	0.56
1:A:284:PRO:HB3	1:A:342:ALA:HB1	1.88	0.56
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.06	0.56
1:B:123:MET:HB2	2:D:168:ARG:HD3	1.87	0.56
3:F:98:MET:HG3	3:F:138:ARG:HG2	1.88	0.56
2:D:192:MET:HA	2:D:192:MET:HE2	1.88	0.56
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.40	0.56
3:F:146:ASN:HB3	3:F:149:ASP:OD2	2.06	0.55
1:A:171:ALA:O	1:A:175:ARG:HB3	2.06	0.55
2:D:324:TRP:C	2:D:327:PRO:HD2	2.30	0.55
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.88	0.55
2:D:262:ARG:HA	2:D:266:GLN:HB3	1.87	0.55
1:B:109:PHE:O	1:B:112:VAL:HG12	2.07	0.55
1:B:230:GLU:C	1:B:233:PRO:HD2	2.32	0.55
3:F:19:ILE:HD12	3:F:19:ILE:C	2.32	0.55
1:B:403:ILE:HD13	1:B:515:LEU:HD13	1.89	0.55
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.71	0.55
1:A:435:THR:HG22	1:A:437:ARG:HE	1.71	0.55
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.89	0.55
2:C:211:THR:O	2:C:214:PRO:HD2	2.07	0.55
1:A:435:THR:HG21	1:A:437:ARG:HH21	1.73	0.54
1:B:137:TYR:O	1:B:141:VAL:HG23	2.08	0.54
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.90	0.54
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.88	0.54
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.72	0.54
1:B:403:ILE:HD11	1:B:507:TRP:CZ3	2.43	0.54
3:E:4:LEU:O	3:E:4:LEU:HG	2.07	0.54
2:D:157:TYR:O	2:D:160:PHE:HB3	2.07	0.54
1:B:227:ASN:ND2	1:B:295:LYS:H	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LYS:HA	1:A:189:SER:HB2	1.89	0.54
2:C:270:PRO:HB3	2:D:270:PRO:CB	2.21	0.54
1:A:155:ASN:HD22	1:A:168:HIS:CD2	2.16	0.54
2:D:143:GLU:O	2:D:147:ARG:HB3	2.08	0.54
2:D:262:ARG:O	2:D:266:GLN:HB3	2.08	0.54
1:B:402:PHE:O	1:B:403:ILE:HD12	2.08	0.53
2:D:224:TYR:O	2:D:227:ALA:N	2.42	0.53
1:B:110:LEU:O	1:B:114:GLU:HG2	2.09	0.53
2:C:146:ASN:O	2:C:214:PRO:HG3	2.09	0.53
3:E:46:SER:OG	3:E:48:GLU:HG2	2.09	0.53
1:A:382:HIS:O	1:A:386:ILE:HG12	2.08	0.53
1:B:208:GLY:O	1:B:213:THR:HG23	2.08	0.53
1:A:160:LYS:HA	2:C:33:ASN:HB2	1.90	0.53
1:A:184:MET:HE2	1:A:188:PHE:CB	2.29	0.53
1:B:205:GLN:HA	1:B:209:GLU:HB2	1.91	0.53
2:D:54:VAL:O	2:D:55:TYR:HB2	2.09	0.53
2:D:141:ARG:HD2	2:D:204:VAL:HG21	1.91	0.53
1:B:403:ILE:HD13	1:B:515:LEU:CD1	2.39	0.53
2:C:146:ASN:HD21	2:C:197:ARG:NH2	2.01	0.53
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.90	0.53
2:C:140:TRP:NE1	2:C:145:ILE:HD11	2.25	0.52
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.91	0.52
1:A:118:ILE:HD13	1:A:145:ILE:HG12	1.91	0.52
2:C:211:THR:C	2:C:214:PRO:HD2	2.34	0.52
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.75	0.52
1:B:310:TYR:CZ	1:B:336:LYS:HD2	2.45	0.52
2:D:332:LEU:HB3	2:D:384:VAL:HG13	1.91	0.52
2:D:313:ASN:HB3	2:D:317:MET:HE2	1.92	0.52
3:E:109:LYS:HE2	6:E:274:HOH:O	2.09	0.52
1:B:48:THR:O	3:F:137:THR:HG23	2.10	0.52
1:B:96:HIS:HB2	2:D:20:ILE:CD1	2.39	0.52
3:E:146:ASN:HB3	3:E:149:ASP:OD2	2.10	0.52
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.91	0.51
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.92	0.51
6:A:2832:HOH:O	3:E:144:ASN:HB3	2.10	0.51
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.09	0.51
1:A:230:GLU:C	1:A:233:PRO:HD2	2.35	0.51
1:B:490:SER:OG	2:D:32:ASN:HB2	2.10	0.51
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.45	0.51
2:C:228:ARG:O	2:C:232:GLU:HG3	2.10	0.51
2:C:306:ASP:O	2:C:310:SER:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:377:ARG:HG2	6:C:593:HOH:O	2.09	0.51
3:F:130:ASP:O	3:F:133:ARG:HG2	2.10	0.51
1:A:108:ASN:HD21	1:A:175:ARG:NE	2.08	0.51
1:A:355:PRO:HG2	1:A:403:ILE:HD13	1.91	0.51
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.46	0.51
1:B:202:LEU:HD22	1:B:206:LEU:CD2	2.40	0.51
1:B:216:LEU:HA	1:B:308:TRP:CH2	2.46	0.51
2:D:336:MET:HE2	2:D:356:LEU:HD11	1.91	0.51
2:D:98:HIS:HD2	2:D:297:ASP:OD1	1.93	0.51
2:D:385:LEU:C	2:D:387:GLY:H	2.19	0.51
2:C:235:TRP:CD1	2:C:235:TRP:C	2.89	0.51
1:A:29:HIS:CD2	1:A:61:LYS:HA	2.47	0.50
1:A:108:ASN:HD21	1:A:175:ARG:NH2	2.09	0.50
1:B:403:ILE:HD11	1:B:507:TRP:HZ3	1.76	0.50
2:D:77:HIS:CG	3:F:140:MET:HG2	2.46	0.50
2:D:167:ALA:O	2:D:176:ARG:NH1	2.44	0.50
1:A:83:GLN:HB3	1:B:77:ARG:HH12	1.76	0.50
1:A:138:LEU:HD22	2:C:160:PHE:CZ	2.46	0.50
2:C:102:LEU:HD13	2:C:290:ILE:HG23	1.91	0.50
1:B:192:PHE:O	1:B:200:CYS:HB3	2.12	0.50
1:B:206:LEU:HD23	1:B:271:LEU:HD13	1.93	0.50
1:B:198:VAL:O	1:B:202:LEU:HG	2.11	0.50
1:B:461:PRO:HG2	3:F:159:ARG:CZ	2.41	0.50
2:C:179:LEU:HD12	2:C:182:TRP:CZ3	2.45	0.50
1:A:65:LYS:HD2	2:C:117:TRP:HB2	1.94	0.50
1:B:202:LEU:HD22	1:B:206:LEU:HD22	1.94	0.50
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.91	0.50
1:A:182:LYS:O	2:C:73:THR:HG21	2.12	0.50
1:B:360:ARG:HG2	1:B:498:GLN:HB2	1.94	0.50
2:D:145:ILE:O	2:D:149:TRP:HB3	2.12	0.50
2:D:260:VAL:O	2:D:265:PHE:HD1	1.94	0.50
2:D:323:LYS:HB2	3:F:78:ARG:NH1	2.25	0.50
1:A:184:MET:HE1	1:A:282:PHE:CZ	2.47	0.50
2:D:152:PHE:O	2:D:155:ASN:HB3	2.12	0.50
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.95	0.49
1:B:52:MET:HE2	1:B:133:GLN:HE22	1.77	0.49
1:B:186:ARG:HA	2:D:73:THR:OG1	2.12	0.49
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.92	0.49
2:D:329:ILE:CD1	2:D:380:ILE:HG23	2.43	0.49
2:D:357:TYR:CE2	2:D:381:VAL:HG21	2.47	0.49
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.94	0.49
1:A:53:ALA:HB3	1:A:56:THR:OG1	2.13	0.49
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.20	0.49
2:C:156:GLU:OE2	2:C:156:GLU:HA	2.13	0.49
3:F:22:LEU:HD11	3:F:31:MET:SD	2.52	0.49
1:A:186:ARG:HD3	1:A:186:ARG:C	2.37	0.49
1:B:204:LEU:HG	1:B:205:GLN:HG3	1.94	0.49
2:D:339:PHE:CE2	2:D:352:ILE:HD12	2.48	0.49
2:D:340:ALA:HB2	2:D:389:LYS:HG2	1.94	0.49
2:D:277:THR:HB	2:D:278:PRO:HD3	1.95	0.49
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.48	0.48
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.94	0.48
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.48	0.48
1:A:184:MET:HE3	1:A:184:MET:HA	1.95	0.48
1:B:50:TYR:CD2	1:B:257:ILE:HD12	2.48	0.48
1:B:401:GLY:HA2	1:B:515:LEU:HD21	1.95	0.48
2:D:228:ARG:HG2	2:D:228:ARG:HH11	1.78	0.48
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.13	0.48
1:B:369:MET:HE2	1:B:379:TRP:HH2	1.77	0.48
3:F:24:THR:HG22	3:F:26:GLU:HB3	1.95	0.48
1:A:81:SER:OG	1:B:84:ASP:HB3	2.14	0.48
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.95	0.48
3:E:12:ARG:O	3:E:16:VAL:HG23	2.14	0.48
3:F:95:VAL:HG12	3:F:99:ASN:ND2	2.29	0.48
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.49	0.48
2:C:111:LYS:O	2:C:115:GLU:HG3	2.13	0.48
2:C:266:GLN:NE2	2:D:132:GLN:OE1	2.47	0.48
1:B:162:GLY:HA3	6:B:2789:HOH:O	2.14	0.47
3:F:55:TRP:CZ2	3:F:59:LYS:HE2	2.49	0.47
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.44	0.47
2:D:376:ASP:OD1	2:D:379:GLN:HB2	2.14	0.47
1:B:206:LEU:HD11	1:B:321:LEU:CD1	2.44	0.47
2:D:54:VAL:HG12	2:D:55:TYR:CD2	2.49	0.47
2:D:226:SER:HB2	2:D:334:ASP:CG	2.40	0.47
1:B:515:LEU:HD21	6:B:2831:HOH:O	2.14	0.47
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.15	0.47
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.80	0.47
1:B:413:HIS:HD2	1:B:428:SER:OG	1.97	0.47
1:A:120:ALA:HA	1:A:193:ILE:HG22	1.95	0.47
1:B:354:TRP:CH2	1:B:499:PRO:HD3	2.50	0.47
1:A:159:ALA:O	2:C:33:ASN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:GLN:HG3	1:B:246:HIS:NE2	2.29	0.47
2:D:208:ASP:OD1	2:D:210:SER:HB3	2.14	0.47
3:F:32:LEU:HD13	3:F:60:LEU:HB3	1.96	0.47
1:A:206:LEU:HB2	6:A:2863:HOH:O	2.15	0.47
2:D:235:TRP:CD1	2:D:235:TRP:C	2.90	0.47
2:D:357:TYR:CD2	2:D:381:VAL:HG21	2.49	0.47
1:A:279:GLN:HG2	1:A:283:THR:OG1	2.15	0.47
1:B:323:LYS:HE2	1:B:324:TYR:CZ	2.50	0.47
3:F:19:ILE:HG21	3:F:60:LEU:HD12	1.97	0.47
1:A:196:ASP:HB2	3:E:140:MET:SD	2.55	0.46
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.50	0.46
1:B:24:ASN:OD1	1:B:27:GLU:HG3	2.14	0.46
1:B:310:TYR:CE1	1:B:336:LYS:HD2	2.50	0.46
1:B:466:CYS:HB2	2:D:73:THR:HA	1.96	0.46
2:C:75:LYS:HB3	2:C:80:ARG:O	2.14	0.46
1:A:435:THR:HG23	3:E:167:GLN:O	2.15	0.46
1:B:30:ARG:HG2	1:B:30:ARG:HH11	1.80	0.46
1:B:190:ASP:HB3	2:D:74:GLN:O	2.16	0.46
1:B:227:ASN:HD21	1:B:296:PHE:H	1.63	0.46
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.98	0.46
2:D:310:SER:O	2:D:314:ARG:HG3	2.15	0.46
1:A:185:LYS:CA	1:A:189:SER:HB2	2.45	0.46
1:B:43:ARG:HD2	1:B:43:ARG:O	2.16	0.46
1:B:103:MET:HE2	1:B:232:THR:OG1	2.15	0.46
1:B:113:GLY:HA3	1:B:188:PHE:CD2	2.50	0.46
3:F:23:ASN:C	3:F:23:ASN:HD22	2.24	0.46
2:C:98:HIS:CD2	2:C:297:ASP:OD1	2.68	0.46
1:A:306:ASP:O	1:A:310:TYR:HB2	2.16	0.46
1:B:56:THR:HG21	1:B:133:GLN:OE1	2.16	0.46
1:B:146:ARG:HG2	1:B:150:GLN:OE1	2.14	0.46
2:D:153:LEU:C	2:D:153:LEU:CD1	2.89	0.46
1:A:175:ARG:HG2	1:A:176:THR:N	2.28	0.46
2:D:16:MET:O	2:D:20:ILE:HG12	2.15	0.46
1:B:113:GLY:HA2	1:B:188:PHE:HB3	1.98	0.46
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.51	0.46
2:D:224:TYR:O	2:D:225:LYS:C	2.59	0.46
2:D:324:TRP:O	2:D:327:PRO:HD2	2.15	0.46
1:A:513:LYS:O	1:A:515:LEU:N	2.49	0.45
1:B:140:GLN:HG3	1:B:246:HIS:CD2	2.51	0.45
3:F:151:PRO:HB2	3:F:153:GLU:OE1	2.15	0.45
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.51	0.45
3:F:36:ARG:HA	3:F:40:THR:HG23	1.98	0.45
3:F:39:HIS:CD2	3:F:49:LEU:HD12	2.51	0.45
1:B:165:PRO:HD2	2:D:30:ASP:HB3	1.99	0.45
2:C:266:GLN:HB2	2:C:281:ILE:HG21	1.98	0.45
1:A:83:GLN:HB3	1:B:77:ARG:NH1	2.31	0.45
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.50	0.45
1:B:216:LEU:HA	1:B:308:TRP:HH2	1.81	0.45
2:C:275:ASN:C	2:C:278:PRO:HD2	2.41	0.45
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.98	0.45
1:B:125:TRP:CD1	1:B:125:TRP:C	2.95	0.45
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.98	0.45
2:C:98:HIS:HD2	2:C:297:ASP:OD1	1.99	0.45
2:D:47:THR:OG1	2:D:50:GLU:HG3	2.16	0.45
1:B:90:ASN:HD22	1:B:90:ASN:HA	1.60	0.45
2:D:339:PHE:O	2:D:342:LEU:HB2	2.16	0.45
2:D:381:VAL:O	2:D:385:LEU:HB2	2.17	0.45
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.98	0.45
2:D:336:MET:C	2:D:338:LEU:H	2.24	0.45
1:A:268:ASN:HD21	1:A:327:GLU:H	1.65	0.45
1:B:32:LEU:HD21	1:B:135:ASN:HB2	1.99	0.44
1:B:292:TYR:OH	1:B:344:HIS:CD2	2.69	0.44
3:F:153:GLU:CD	3:F:153:GLU:N	2.73	0.44
1:A:227:ASN:HD21	1:A:296:PHE:H	1.64	0.44
1:A:390:TRP:HE1	1:A:407:TRP:CG	2.35	0.44
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.51	0.44
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.52	0.44
1:B:459:ALA:C	1:B:461:PRO:HD3	2.42	0.44
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.51	0.44
2:D:153:LEU:HB3	2:D:193:ILE:HG21	1.99	0.44
3:F:40:THR:C	3:F:41:THR:HG23	2.42	0.44
3:F:86:ASP:O	3:F:89:SER:HB2	2.17	0.44
1:A:206:LEU:HD11	1:A:321:LEU:HD11	1.98	0.44
2:C:143:GLU:O	2:C:147:ARG:HB3	2.18	0.44
2:D:312:TYR:O	2:D:316:VAL:HG23	2.18	0.44
1:A:113:GLY:HA2	1:A:188:PHE:O	2.18	0.44
1:A:303:LYS:HE3	1:A:303:LYS:HB2	1.85	0.44
1:A:305:TRP:CE2	1:A:309:VAL:HG21	2.52	0.44
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.53	0.44
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.48	0.44
1:B:193:ILE:HB	2:D:168:ARG:CZ	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:ASP:HA	1:B:398:PRO:HD3	1.82	0.44
2:D:111:LYS:O	2:D:115:GLU:HG3	2.17	0.44
1:B:460:GLU:OE1	1:B:463:ARG:HD3	2.18	0.43
2:D:155:ASN:ND2	2:D:252:TYR:OH	2.45	0.43
1:B:50:TYR:CD1	1:B:50:TYR:N	2.86	0.43
1:B:105:VAL:O	1:B:109:PHE:HB2	2.18	0.43
1:B:291:GLU:OE1	1:B:343:HIS:CE1	2.70	0.43
2:C:90:LEU:HD13	2:C:303:LEU:HD13	2.00	0.43
2:D:336:MET:HE1	2:D:356:LEU:HD11	1.99	0.43
1:B:460:GLU:N	1:B:461:PRO:HD3	2.34	0.43
2:D:197:ARG:HB3	2:D:197:ARG:NH1	2.34	0.43
1:B:143:ASP:CG	1:B:245:ARG:HH21	2.26	0.43
2:C:54:VAL:O	2:C:55:TYR:HB2	2.18	0.43
1:B:138:LEU:HD22	2:D:160:PHE:CZ	2.54	0.43
1:A:302:VAL:HG13	1:A:376:TYR:CE2	2.53	0.43
1:B:159:ALA:O	2:D:33:ASN:HB2	2.18	0.43
2:C:153:LEU:C	2:C:153:LEU:HD12	2.44	0.43
3:F:23:ASN:H	3:F:23:ASN:ND2	2.17	0.43
1:B:52:MET:HE2	1:B:133:GLN:NE2	2.33	0.42
3:F:33:LYS:HE3	3:F:117:ALA:CB	2.48	0.42
1:B:124:LEU:HD21	1:B:201:SER:HB2	2.00	0.42
1:B:185:LYS:HA	1:B:189:SER:HB2	2.01	0.42
1:B:186:ARG:HD3	1:B:186:ARG:C	2.44	0.42
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.53	0.42
2:D:332:LEU:HB3	2:D:384:VAL:CG1	2.48	0.42
1:A:113:GLY:HA3	1:A:188:PHE:CD2	2.55	0.42
2:D:357:TYR:O	2:D:361:ASP:HB2	2.19	0.42
3:E:165:HIS:CE1	3:E:167:GLN:HG3	2.54	0.42
1:A:179:PRO:HB3	1:A:469:ILE:HD13	2.00	0.42
1:B:123:MET:HE1	1:B:200:CYS:SG	2.59	0.42
1:B:165:PRO:HG3	6:B:2823:HOH:O	2.19	0.42
1:B:207:VAL:HG11	1:B:275:PHE:HA	2.02	0.42
2:C:115:GLU:HB3	2:D:115:GLU:HB3	2.01	0.42
2:D:340:ALA:CA	2:D:389:LYS:HE2	2.33	0.42
1:A:90:ASN:HD22	1:A:90:ASN:HA	1.56	0.42
1:A:175:ARG:HG3	1:A:181:TRP:CG	2.54	0.42
1:B:49:LYS:HD3	3:F:140:MET:CB	2.47	0.42
2:D:169:GLU:O	2:D:170:ALA:C	2.60	0.42
2:D:223:VAL:HA	2:D:334:ASP:O	2.20	0.42
1:A:187:VAL:HG12	1:A:277:THR:HG22	2.01	0.42
1:A:223:TRP:CZ3	1:A:297:LYS:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:269:ALA:N	2:D:270:PRO:CD	2.83	0.42
2:C:243:GLU:OE1	2:C:323:LYS:NZ	2.46	0.42
3:E:33:LYS:NZ	6:E:229:HOH:O	2.48	0.42
1:A:302:VAL:HG23	1:A:303:LYS:H	1.85	0.42
1:A:323:LYS:HE2	1:A:324:TYR:CZ	2.54	0.42
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.20	0.42
2:C:33:ASN:N	2:C:33:ASN:HD22	2.16	0.42
1:A:108:ASN:O	1:A:111:GLU:HB3	2.20	0.42
1:A:279:GLN:HE21	1:A:279:GLN:HB3	1.73	0.42
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.54	0.42
1:B:451:GLN:HG2	6:B:2845:HOH:O	2.18	0.42
2:C:176:ARG:HB2	2:C:176:ARG:NH1	2.35	0.41
2:D:342:LEU:HD13	2:D:346:THR:HG21	2.02	0.41
3:F:73:ASN:O	3:F:74:GLU:C	2.63	0.41
1:B:63:ILE:HA	2:D:191:GLN:HE22	1.85	0.41
1:A:125:TRP:CD1	1:A:125:TRP:C	2.98	0.41
1:A:149:HIS:CE1	2:C:105:TRP:HB2	2.56	0.41
1:A:260:ASP:HA	1:A:261:PRO:HD3	1.95	0.41
1:B:108:ASN:ND2	1:B:175:ARG:HH11	2.14	0.41
2:C:336:MET:HE2	2:C:336:MET:HA	2.01	0.41
2:D:63:ILE:O	2:D:64:ALA:C	2.63	0.41
3:F:23:ASN:HD22	3:F:23:ASN:H	1.69	0.41
1:B:259:ASN:HD22	1:B:259:ASN:HA	1.70	0.41
2:D:95:TRP:CE2	2:D:171:LEU:HD12	2.56	0.41
3:F:36:ARG:CZ	3:F:119:LYS:HB3	2.51	0.41
1:A:118:ILE:HG21	2:C:176:ARG:HD3	2.02	0.41
1:A:365:ASP:OD2	1:A:365:ASP:C	2.63	0.41
1:B:163:GLN:HG2	6:B:2675:HOH:O	2.21	0.41
2:D:146:ASN:HB2	2:D:207:PHE:CZ	2.56	0.41
2:D:388:LEU:O	2:D:389:LYS:C	2.64	0.41
3:F:154:GLU:HG3	3:F:158:GLN:NE2	2.35	0.41
1:A:119:ALA:HB1	2:C:168:ARG:HD2	2.02	0.41
1:A:253:THR:O	1:A:257:ILE:HG12	2.20	0.41
1:A:520:LYS:HB3	1:A:520:LYS:NZ	2.36	0.41
1:B:334:ASP:O	1:B:337:GLN:HB3	2.20	0.41
1:B:444:GLU:HA	1:B:444:GLU:OE2	2.21	0.41
3:F:23:ASN:ND2	3:F:23:ASN:N	2.69	0.41
1:A:52:MET:HA	1:A:256:SER:O	2.21	0.41
1:A:123:MET:HB2	2:C:168:ARG:HD3	2.02	0.41
1:B:413:HIS:CD2	1:B:428:SER:OG	2.74	0.41
3:E:129:LEU:HD23	3:E:129:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:ND2	1:A:175:ARG:HE	2.18	0.41
1:A:109:PHE:HB3	1:A:184:MET:SD	2.61	0.41
1:A:283:THR:HB	1:A:284:PRO:CD	2.50	0.41
1:A:435:THR:HG21	1:A:437:ARG:NE	2.28	0.41
1:A:444:GLU:HG3	1:A:445:MET:N	2.35	0.41
1:B:32:LEU:HD12	1:B:35:PHE:CD2	2.56	0.41
1:B:194:SER:HA	2:D:76:PHE:CE1	2.56	0.41
1:B:202:LEU:CD2	1:B:206:LEU:HD22	2.51	0.41
1:B:232:THR:N	1:B:233:PRO:CD	2.83	0.41
3:F:152:LEU:O	3:F:156:ARG:HG3	2.20	0.41
2:C:376:ASP:HB3	2:C:379:GLN:HB2	2.02	0.41
2:D:228:ARG:O	2:D:232:GLU:HG3	2.21	0.41
3:E:165:HIS:CE1	3:E:167:GLN:HE21	2.30	0.41
1:A:65:LYS:HB3	2:C:117:TRP:CD2	2.56	0.40
1:B:284:PRO:HB3	1:B:342:ALA:HB1	2.04	0.40
2:D:385:LEU:HD12	2:D:385:LEU:HA	1.95	0.40
3:E:40:THR:C	3:E:41:THR:HG23	2.46	0.40
1:A:114:GLU:CD	1:A:147:HIS:HB3	2.47	0.40
1:A:423:VAL:HA	1:A:424:PRO:HD3	1.91	0.40
1:B:30:ARG:HG2	1:B:30:ARG:NH1	2.36	0.40
1:B:305:TRP:CE2	1:B:309:VAL:HG21	2.56	0.40
2:C:146:ASN:ND2	2:C:197:ARG:NH2	2.62	0.40
2:D:187:ILE:O	2:D:191:GLN:HG3	2.21	0.40
3:F:80:LYS:HE3	3:F:84:GLY:HA2	2.01	0.40
1:B:297:LYS:HG2	1:B:371:TRP:CE2	2.56	0.40
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.56	0.40
1:A:307:ARG:HG2	1:A:312:ASP:OD2	2.20	0.40
2:D:213:VAL:N	2:D:214:PRO:HD2	2.37	0.40
2:D:234:LEU:HD13	2:D:248:VAL:HG22	2.04	0.40
2:D:264:PHE:O	2:D:268:LEU:HG	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	508/527 (96%)	482 (95%)	24 (5%)	2 (0%)	30	38
1	B	508/527 (96%)	479 (94%)	25 (5%)	4 (1%)	16	20
2	C	386/389 (99%)	373 (97%)	12 (3%)	1 (0%)	36	46
2	D	386/389 (99%)	354 (92%)	29 (8%)	3 (1%)	16	20
3	E	164/170 (96%)	161 (98%)	3 (2%)	0	100	100
3	F	164/170 (96%)	151 (92%)	9 (6%)	4 (2%)	4	4
All	All	2116/2172 (97%)	2000 (94%)	102 (5%)	14 (1%)	18	23

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	LYS
1	B	311	GLU
2	D	251	VAL
1	B	39	PHE
2	D	64	ALA
2	C	64	ALA
3	F	74	GLU
3	F	87	ALA
1	A	94	ARG
1	A	340	TYR
1	B	94	ARG
3	F	122	ILE
2	D	386	ALA
3	F	5	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	425/442 (96%)	418 (98%)	7 (2%)	55	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	422/442 (96%)	413 (98%)	9 (2%)	47	66
2	C	315/323 (98%)	307 (98%)	8 (2%)	42	60
2	D	312/323 (97%)	307 (98%)	5 (2%)	55	73
3	E	143/147 (97%)	140 (98%)	3 (2%)	47	66
3	F	142/147 (97%)	138 (97%)	4 (3%)	38	56
All	All	1759/1824 (96%)	1723 (98%)	36 (2%)	48	67

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	90	ASN
1	A	125	TRP
1	A	175	ARG
1	A	318	ILE
1	A	467	GLN
1	A	514	ARG
1	B	70	MET
1	B	90	ASN
1	B	125	TRP
1	B	222	GLU
1	B	259	ASN
1	B	279	GLN
1	B	302	VAL
1	B	311	GLU
1	B	523	VAL
2	C	33	ASN
2	C	153	LEU
2	C	173	ASP
2	C	179	LEU
2	C	195	LEU
2	C	266	GLN
2	C	311	ASP
2	C	378	ASP
2	D	4	LEU
2	D	80	ARG
2	D	153	LEU
2	D	173	ASP
2	D	205	PRO
3	E	31	MET

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Mol	Chain	Res	Type
3	E	44	ARG
3	E	60	LEU
3	F	11	THR
3	F	23	ASN
3	F	44	ARG
3	F	164	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	78	GLN
1	A	83	GLN
1	A	90	ASN
1	A	108	ASN
1	A	116	ASN
1	A	168	HIS
1	A	203	ASN
1	A	205	GLN
1	A	214	ASN
1	A	227	ASN
1	A	249	ASN
1	A	259	ASN
1	A	268	ASN
1	A	272	ASN
1	A	273	ASN
1	A	343	HIS
1	A	344	HIS
1	A	412	ASN
1	A	413	HIS
1	A	422	GLN
1	A	439	HIS
1	A	442	ASN
1	A	472	GLN
1	A	516	ASN
1	B	33	GLN
1	B	42	ASN
1	B	78	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	ASN
1	B	116	ASN

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Mol	Chain	Res	Type
1	B	161	ASN
1	B	168	HIS
1	B	205	GLN
1	B	227	ASN
1	B	249	ASN
1	B	259	ASN
1	B	268	ASN
1	B	273	ASN
1	B	279	GLN
1	B	343	HIS
1	B	344	HIS
1	B	382	HIS
1	B	413	HIS
1	B	439	HIS
1	B	451	GLN
1	B	516	ASN
1	B	527	ASN
2	C	33	ASN
2	C	98	HIS
2	C	146	ASN
2	C	161	ASN
2	C	266	GLN
2	C	285	GLN
2	C	301	ASN
2	D	57	GLN
2	D	59	ASN
2	D	98	HIS
2	D	155	ASN
2	D	161	ASN
2	D	285	GLN
2	D	296	GLN
2	D	301	ASN
3	E	23	ASN
3	E	45	ASN
3	E	165	HIS
3	E	167	GLN
3	F	7	HIS
3	F	23	ASN
3	F	45	ASN
3	F	99	ASN
3	F	144	ASN
3	F	158	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	FPN	B	2667	-	8,8,8	2.48	5 (62%)	10,10,10	2.12	3 (30%)
5	FPN	A	2666	-	8,8,8	2.63	5 (62%)	10,10,10	2.16	3 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FPN	B	2667	-	-	-	0/1/1/1
5	FPN	A	2666	-	-	-	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2666	FPN	C6-C5	4.15	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2667	FPN	C6-C5	4.04	1.45	1.38
5	A	2666	FPN	C3-C2	3.65	1.44	1.38
5	B	2667	FPN	C3-C2	3.14	1.43	1.38
5	A	2666	FPN	C3-C4	2.67	1.42	1.37
5	B	2667	FPN	C3-C4	2.65	1.42	1.37
5	A	2666	FPN	C2-C1	2.61	1.43	1.39
5	B	2667	FPN	C5-C4	2.53	1.42	1.37
5	A	2666	FPN	C5-C4	2.47	1.42	1.37
5	B	2667	FPN	C2-C1	2.45	1.43	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2666	FPN	C3-C2-C1	-3.64	116.03	119.88
5	B	2667	FPN	C6-C1-C2	3.59	125.48	119.77
5	B	2667	FPN	C3-C2-C1	-3.55	116.12	119.88
5	A	2666	FPN	C6-C1-C2	3.54	125.41	119.77
5	A	2666	FPN	C5-C6-C1	-3.21	116.48	119.88
5	B	2667	FPN	C5-C6-C1	-3.11	116.59	119.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	510/527 (96%)	0.15	19 (3%)	45	48	21, 39, 68, 80	0
1	B	510/527 (96%)	0.07	17 (3%)	49	51	23, 37, 68, 79	0
2	C	388/389 (99%)	-0.59	0	100	100	17, 26, 41, 61	0
2	D	388/389 (99%)	0.59	24 (6%)	26	28	26, 48, 73, 93	0
3	E	166/170 (97%)	-0.35	3 (1%)	67	69	20, 30, 48, 68	0
3	F	166/170 (97%)	1.09	19 (11%)	10	11	37, 57, 77, 83	0
All	All	2128/2172 (97%)	0.11	82 (3%)	43	45	17, 37, 70, 93	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	4	LEU	3.8
1	A	213	THR	3.7
1	A	433	ALA	3.6
1	A	212	PHE	3.5
3	E	168	SER	3.5
3	F	25	LEU	3.3
1	A	338	ASP	3.2
3	F	71	ALA	3.1
1	A	318	ILE	3.1
1	A	206	LEU	3.1
1	A	19	ALA	3.0
2	D	270	PRO	3.0
2	D	354	ALA	3.0
1	B	188	PHE	2.9
2	D	275	ASN	2.8
1	A	514	ARG	2.8
1	B	206	LEU	2.8
1	B	53	ALA	2.8
1	B	213	THR	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	389	LYS	2.7
2	D	205	PRO	2.7
1	B	23	VAL	2.6
2	D	380	ILE	2.6
2	D	204	VAL	2.6
3	F	19	ILE	2.6
2	D	363	TRP	2.6
1	A	251	TYR	2.6
3	F	75	VAL	2.6
3	F	82	ALA	2.6
2	D	352	ILE	2.6
2	D	338	LEU	2.5
1	A	210	ALA	2.5
1	B	317	TRP	2.5
2	D	384	VAL	2.5
2	D	136	MET	2.5
1	A	248	ALA	2.5
1	B	19	ALA	2.5
3	F	77	PHE	2.5
3	F	127	TYR	2.4
1	B	20	PRO	2.4
3	F	16	VAL	2.4
1	A	139	ALA	2.4
3	F	72	PHE	2.4
3	F	118	TYR	2.4
2	D	328	THR	2.4
1	A	253	THR	2.3
1	B	52	MET	2.3
1	B	247	MET	2.3
3	E	4	LEU	2.3
3	E	167	GLN	2.3
3	F	60	LEU	2.3
1	B	54	ASN	2.3
3	F	24	THR	2.3
2	D	137	ASN	2.3
2	D	343	PRO	2.3
2	D	206	GLY	2.3
1	A	317	TRP	2.3
1	B	308	TRP	2.3
1	B	265	LYS	2.3
3	F	67	LEU	2.2
2	D	387	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	350	GLU	2.2
2	D	375	ALA	2.2
2	D	329	ILE	2.2
3	F	122	ILE	2.2
1	B	313	TRP	2.2
3	F	79	HIS	2.2
2	D	353	THR	2.2
1	A	308	TRP	2.1
2	D	385	LEU	2.1
1	A	328	SER	2.1
3	F	69	ALA	2.1
3	F	101	ALA	2.1
1	A	316	ILE	2.1
2	D	342	LEU	2.1
1	B	37	TRP	2.1
1	A	435	THR	2.0
2	D	139	THR	2.0
1	A	432	GLY	2.0
1	B	47	ALA	2.0
1	B	210	ALA	2.0
3	F	117	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FPN	B	2667	8/8	0.93	0.10	34,35,37,41	0
5	FPN	A	2666	8/8	0.96	0.08	30,33,36,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FE	B	529	1/1	0.96	0.05	72,72,72,72	0
4	FE	B	528	1/1	0.97	0.07	63,63,63,63	0
4	FE	A	528	1/1	0.98	0.07	63,63,63,63	0
4	FE	A	529	1/1	0.99	0.05	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.